

Trying 3106016892...Open

09/630,270

Welcome to STN International! Enter x:x  
LOGINID:SSSPTAU121BD  
PASSWORD:  
TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Aug 21 CAS patent coverage expanded  
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Substances (PICCS) has been added to CHEMLIST  
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Enter NEWS followed by the item number or name to see news on that  
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FILE 'HOME' ENTERED AT 13:26:11 ON 07 NOV 2000

=> fil reg

FILE 'REGISTRY' ENTERED AT 13:27:34 ON 07 NOV 2000  
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STRUCTURE FILE UPDATES: 6 NOV 2000 HIGHEST RN 301521-88-0  
DICTIONARY FILE UPDATES: 6 NOV 2000 HIGHEST RN 301521-88-0

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT  
for details.

\*\*\* YOU HAVE NEW MAIL \*\*\*

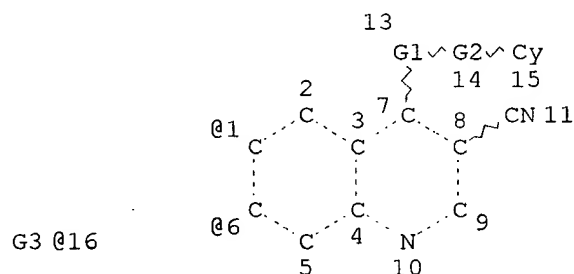
'REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> str

=> d sia

L1 HAS NO ANSWERS

L1 STR



VAR G1=O/N/S

REP G2=(0-1) CH2

VAR G3=O/N

VPA 16-1/6 U

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

=> fil stn guide

'STN' IS AN AMBIGUOUS FILE NAME

STNGUIDE - Descriptive information about STN databases

STNMAIL - STN Electronic Mail Service

Enter the appropriate file name or enter "IGNORE" to continue  
accessing the remaining files of your multiple file entry.

ENTER A FILE NAME OR (IGNORE):stnguide

MULTIFILE PROCESSING IS NOT ALLOWED IN FILE 'STNGUIDE'

The file entered is not valid in multifile processing. Enter "HELP  
DUFILES" to see a list of the valid files.

ENTER A FILE NAME OR (IGNORE):ignore

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'GUIDE' IS NOT A VALID FILE NAME

SESSION CONTINUES IN FILE 'REGISTRY'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> fil stnguide

FILE 'STNGUIDE' ENTERED AT 13:37:37 ON 07 NOV 2000  
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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Oct 27, 2000 (20001027/UP).

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=> fil reg

FILE 'REGISTRY' ENTERED AT 13:56:37 ON 07 NOV 2000  
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TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

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conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT  
for details.

'REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> s 11

SAMPLE SEARCH INITIATED 13:56:45 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 57 TO ITERATE

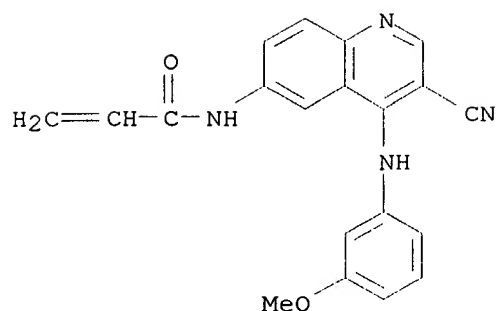
100.0% PROCESSED 57 ITERATIONS 33 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 688 TO 1592  
PROJECTED ANSWERS: 316 TO 1004

L2 33 SEA SSS SAM L1

=> d scan

L2 33 ANSWERS REGISTRY COPYRIGHT 2000 ACS  
IN 2-Propenamide, N-[3-cyano-4-[(3-methoxyphenyl)amino]-6-quinolinyl]- (9CI)  
MF C20 H16 N4 O2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s 11 ful

FULL SEARCH INITIATED 13:57:25 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1041 TO ITERATE

100.0% PROCESSED 1041 ITERATIONS  
SEARCH TIME: 00.00.02

586 ANSWERS

L3 586 SEA SSS FUL L1

=> d 1- reg

YOU HAVE REQUESTED DATA FROM 586 ANSWERS - CONTINUE? Y/(N):y

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L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2000 ACS

2000:628125 Document No. 133:207919 Preparation of 4-amino-quinazoline and quinoline derivatives having an inhibitory effect on signal transduction mediated by tyrosine kinases useful for treating tumoral diseases, lung and respiratory tract diseases. Himmelsbach, Frank; Langkopf, Elke;

Jung, Birgit; Metz, Thomas; Solca, Flavio; Blech, Stefan (Boehringer Ingelheim Pharma K.-G., Germany). PCT Int. Appl. WO 2000051991 A1 20000908, 232

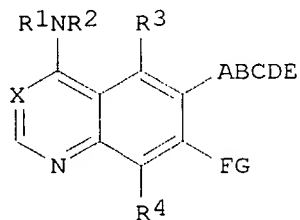
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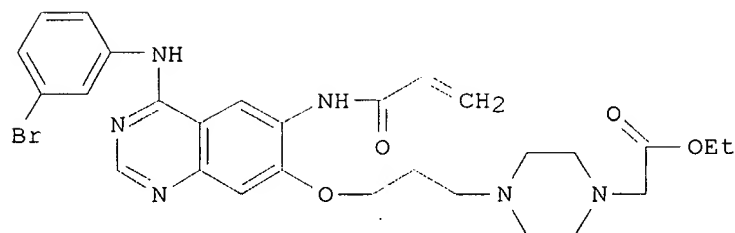
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TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-EP1496 20000224. PRIORITY: DE 1999-19908567 19990227; DE 1999-19911366 19990315; DE 1999-19928306 19990621; US 1999-PV149329 19990817; DE 1999-19954816 19991113.

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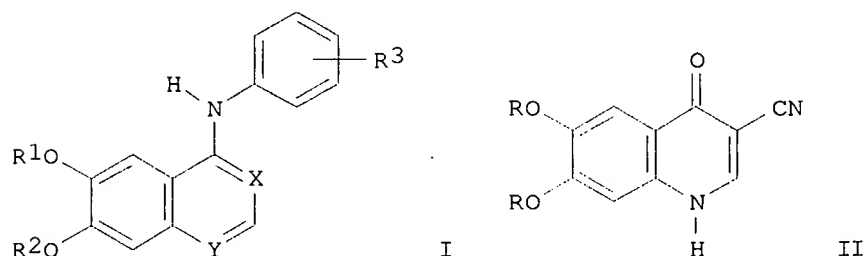
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AB Title compds. [I; R1 = H, C1-C4-alkyl; R2 = (un)substituted Ph, benzyl, 1-phenylethyl; R3, R4 independently = H, F, Cl, CH3O, CH3OCH2, (CH3)2NCH2, (CH3CH2)2NCH2, pyrrolidino, piperidino, morpholino; X = C(CN), N; A = O, NH, (C1-C4)-alkylN; B = CO, SO2; C = 1,3-allenylene, 1,1-vinylene, 1,2-vinylene, 1,3-butadien-1,4-ylene, with CH3, CF3 substitution; D = alkylene, CO-alkylene, SO2-alkylene; CO, SO2; E = HOCO(CH2)nNR5, (HO)2P(:O)(CH2)nNR5; n = 1-6; R5 = H, alkyl], tautomers, stereoisomers, and physiol. acceptable salts are prepd. and having valuable pharmacol. properties, particularly an inhibiting effect on signal transduction mediated by tyrosine kinases. Title compds. are useful for treating tumoral diseases, diseases of the lungs and respiratory tract. Thus, the title compd. II was prepd. and tested by Cell Titer 96TM Aq. Nonradioactive Cell Proliferation Assay.

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2000 ACS  
2000:543462 Document No. 133:237831 4-Anilino-6,7-dialkoxyquinoline-3-carbonitrile inhibitors of epidermal growth factor receptor kinase and their bioisosteric relationship to the 4-anilino-6,7-dialkoxyquinazoline inhibitors. Wissner, Allan; Berger, Dan M.; Boschelli, Diane H.; Floyd, M. Brawner Jr.; Greenberger, Lee M.; Gruber, Brian C.; Johnson, Bernard D.; Mamuya, Nellie; Nilakantan, Ramaswamy; Reich, Marvin F.; Shen, Ru; Tsou, Hwei-Ru; Upeslacis, Erik; Wang, Yu Fen; Wu, Biqi; Ye, Fei; Zhang,



GI



AB The synthesis and SAR (structure-activity relationship) of a series of 4-anilino-6,7-dialkoxyquinoline-3-carbonitrile inhibitors of epidermal growth factor receptor (EGF-R) kinase, I [R1 = Me, Et, MeOCH2, MeO(CH2)2, R2 = H, Et, MeO(CH2)2, etc.; R1R2 = CH2, CH2CH2, (CH2)3, R3 = 3-Br, 4-F, 3-NHAc, etc., X = CCO2Et, N, CCN, etc., Y = N, CCN], are described.

Condensation of 3,4-dialkoxyanilines with Et

(ethoxymethylene)cyanoacetate

followed by thermal cyclization gave, regiospecifically,

6,7-dialkoxy-4-oxo-1,4-dihydroquinoline-3-carbonitriles, e.g. II (R = Et, Me). Chlorination (POCl3) followed by the reaction with substituted anilines furnished the 4-anilino-6,7-dialkoxyquinoline-3-carbonitrile inhibitors of EGF-R kinase. An alternate synthesis of these compds. starts with a Me 3,4-dialkoxybenzoate. Nitration followed by redn. (Fe, NH4Cl, MeOH-H2O) gave a Me 2-amino-4,5-dialkoxybenzoate. Amidine

formation using DMF-acetal followed by cyclization using LiCH2CN furnished

a 6,7-dialkoxy-4-oxo-1,4-dihydroquinoline-3-carbonitrile, which was transformed as before. Compds. contg. acid, ester, amide, carbinol, and aldehyde groups at the 3-position of the quinoline ring were also prepd. for comparison, as were several 1-anilino-6,7-dimethoxyisoquinoline-4-carbonitriles. The compds. were evaluated for their ability to inhibit the autophosphorylation of the catalytic domain of EGF-R. The SAR of these inhibitors with respect to the nature of the 6,7-alkoxy groups, the aniline substituents, and the substituent at the 3-position was studied. The compds. were further evaluated for their ability to inhibit the

growth

of cell lines that overexpress EGF-R or HER-2. It was found that 4-anilinoquinoline-3-carbonitriles are effective inhibitors of EGF-R kinase with activity comparable to the 4-anilinoquinazoline-based inhibitors. A new homol. model of EGF-R kinase was constructed based on the X-ray structures of Hck and FGF receptor-1 kinase. The model

suggests

that with the quinazoline-based inhibitors, the N3 atom is

hydrogen-bonded

to a water mol. which, in turn, interacts with Thr 830. It is proposed that the quinoline-3-carbonitriles bind in a similar manner where the water mol. is displaced by the cyano group which interacts with the same Thr residue.

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2000 ACS

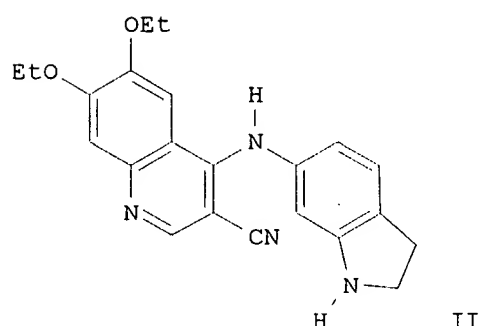
2000:227652 Document No. 132:265101 Preparation of 3-cyanoquinolines as protein tyrosine kinase inhibitors. Wissner, Allan; Tsou, Hwei-Ru;

Berger, Dan Maarten; Floyd, Middleton Brawner, Jr.; Hamann, Philip Ross; Zhang, Nan; Salvati, Mark Ernest; Frost, Philip (American Cyanamid Company, USA). PCT Int. Appl. WO 2000018761 A1 20000406, 195 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA,

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CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US22054 19990922. PRIORITY: US 1998-162802 19980929.

GI



AB X(CH<sub>2</sub>)<sub>n</sub>ZZ<sub>1</sub>CN [I; X = (un)substituted bicyclic (hetero)aryl or LTA; A = (un)substituted phenylene, -pyridinediyl, -pyrimidinediyl; T = O, S, (alkyl)imino(alkylene), oxyalkylene, etc.; Z = O, S, (alkyl or alkanoyl)imino; Z<sub>1</sub> = 2-unsubstituted-5,6,7,8-(un)substituted quinoline-4,3-diyl; n = 0 or 1] were prep'd. Thus, Me 2-amino-4,5-diethoxybenzoate was N-condensed with HCNMe<sub>2</sub>/POCl<sub>3</sub> and the product cyclocondensed with MeCN to give, after POCl<sub>3</sub> treatment, 4-chloro-6,7-diethoxyquinoline-3-carbonitrile which was aminated by 6-aminoindoline to give title comp'd II. Data for biol. activity of I were given.

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2000 ACS

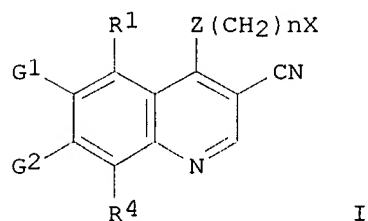
2000:227636 Document No. 132:265100 Preparation of substituted 3-cyanoquinolines as protein tyrosine kinases inhibitors. Wissner, Allan;

Tsou, Hwei-Ru; Berger, Dan Maarten; Floyd, Middleton Brawner, Jr.; Hamann,

Philip Ross; Zhang, Nan; Frost, Philip (American Cyanamid Company, USA). PCT Int. Appl. WO 2000018740 A1 20000406, 164 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US22056 19990922. PRIORITY: US 1998-162289

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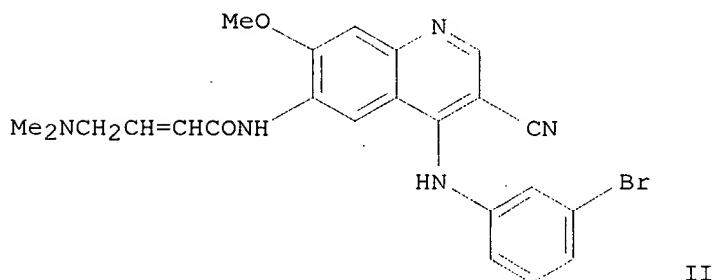
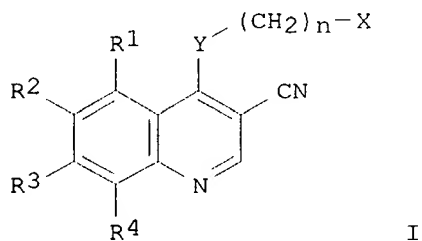
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AB The title compds. I [X = cycloalkyl, pyridinyl, pyrimidinyl, etc.; Z = NH, O, S, NR; G1, G2, R1, R4 = H, halo, alkyl, alkynyl, etc.; n = 0,1], protein tyrosine kinase inhibitors, were prepd. E.g., 4-(2-methoxyethoxy)but-2-ynoic acid [4-(3-bromophenylamino)-3-cyanoquinolin-6-yl]amide was prepd. I are useful as antineoplastic agents.

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2000 ACS  
 1999:794373 Document No. 132:35620 Preparation of substituted 3-cyanoquinolines as inhibitors of growth factor receptor protein tyrosine kinases (PTK). Wissner, Allan; Johnson, Bernard D.; Reich, Marvin F.; Floyd, Middleton B. , Jr.; Kitchen, Douglas B.; Tsou, Hwei-ru (American Cyanamid Co., USA). U.S. US 6002008 A 19991214, 80 pp. (English). CODEN: USXXAM. APPLICATION: US 1998-49718 19980327. PRIORITY: US 1997-41963 19970403.

GI



AB This invention provides compds. having the formula (I; wherein: X is cycloalkyl which may be optionally substituted; or is a pyridinyl, pyrimidinyl, or Ph ring; wherein the pyridinyl, pyrimidinyl, or Ph ring may be optionally substituted; n is 0-1; Y is NH, O, S, or NR; R is alkyl of 1-6 carbon atoms; R1, R2, R3, and R4 are each, independently,

hydrogen,

halogen, alkyl, alkenyl, alkynyl, alkenyloxy, alkynyloxy, hydroxymethyl, halomethyl, alkanoyloxy, alkenoyloxy, alkynyloxy, alkanoyloxymethyl, alkenoyloxymethyl, alkynyloxymethyl, alkoxy, alkylthio, alkylsulphanyl, alkylsulfonyl, alkylsulfonamido, alkenylsulfonamido, alkynylsulfonamido, hydroxy, trifluoromethyl, cyano, nitro, carboxy, carboalkoxy, carboalkyl, phenoxy, Ph, thiophenoxy, benzyl, amino, hydroxyamino, alkoxyamino, alkylamino, dialkylamino, aminoalkyl, N-alkylaminoalkyl, N,N-dialkylaminoalkyl, phenylamino, benzylamino, etc.; R5 is alkyl which may be optionally substituted, or Ph which may be optionally substituted; R6 is hydrogen, alkyl, or alkenyl; R7 is chloro

or

bromo; R8 is hydrogen, alkyl, aminoalkyl, N-alkylaminoalkyl, N,N-dialkylaminoalkyl, N-cycloalkylaminoalkyl, N-cycloalkyl-N-alkylaminoalkyl, N,N-dicycloalkylaminoalkyl, morpholino-N-alkyl, piperidino-N-alkyl, N-alkyl-piperidino-N-alkyl, azacycloalkyl-N-alkyl, hydroxyalkyl, alkoxyalkyl, carboxy, carboalkoxy, Ph, carboalkyl, chloro, fluoro, or bromo; Z is amino, hydroxy, alkoxy, alkylamino, dialkylamino). The compds. of the present invention inhibit the action of certain growth factor receptor protein tyrosine kinases (PTK) thereby inhibiting the abnormal growth of certain cell types. They are therefore useful for the treatment of certain diseases that are the result of deregulation of

these

PTKs, in particular as anti-cancer agents for the treatment of cancers expressing epidermal growth factor receptor (EGFR), mitogen activated protein kinase (MAPK), epithelial kinase (ECK), and kinase insert domain contg. receptor (KDR) in mammals and for the treatment of polycystic kidney disease in mammals. Thus, To a mixt. of 1.9 g (5.1 mmol) of 4-[(3-bromophenyl)amino]-7-methoxy-6-amino-3-quinolinecarbonitrile and

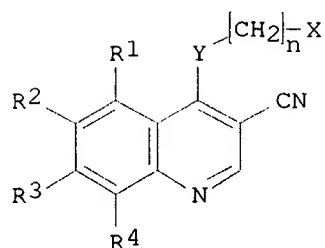
5.3

mL (31 mmol) of Hunig's base in 110 mL of dry THF at 0.degree. C., with stirring, was added a THF soln. contg. 5.7 g (31 mmol) of 4-bromocrotonyl chloride dropwise. The mixt. was stirred for addnl. 0.5 h. After addn. 100 mL of satd. sodium chloride soln. was added to the reaction mixt., then it was extd. with Et acetate. The Et acetate soln. was dried over sodium sulfate and then was added to 40 mL of di-Me amine soln. (2.0 M in THF) at 0.degree. dropwise and stirred an addnl. 0.5 h to give 4-Dimethylamino-but-2-enoic acid [4-(3-bromo-phenylamino)-3-cyano-7-methoxy-quinolin-6-yl]amide (II). II showed IC50 of 0.000008 .mu.M against epidermal growth factor receptor kinase.

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2000 ACS

1998:682233 Document No. 129:302564 Preparation of substituted 3-cyanoquinolines as inhibitors of protein tyrosine kinase. Wissner, Allan; Johnson, Bernard Dean; Reich, Marvin Fred; Floyd, Middleton Brawner, Jr.; Kitchen, Douglas B.; Tsou, Hwei-ru (American Cyanamid Co., USA). PCT Int. Appl. WO 9843960 A1 19981008, 223 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US6480 19980402. PRIORITY: US 1997-826604 19970403.

GI



AB The title compds. [I; X = (un)substituted cycloalkyl, pyridinyl, pyrimidinyl, Ph; n = 0-1; Y = NH, O, S, NR; R = C1-6 alkyl; R1-R4 = H, halo, alkyl, etc. (with the proviso that when Y = NH; R1-R4 = H; n = 0; X is not 2-methylphenyl)], inhibitors of protein tyrosine kinase which are useful in treating, inhibiting the growth of, or eradicating a neoplasm. which expresses EGFR, MAPK, ECK or KDR, and in treating polycystic kidney disease, were prepd. Thus, treatment of 2-butynoic acid with iso-Bu chloroformate and N-methylmorpholine in THF followed by the addn. of this soln. of the mixed anhydride to a soln. of 6-amino-4-[(3-bromophenyl)amino]-7-methoxy-3-quinolinecarbonitrile (prepn. described)

in THF over a 24 h period afforded I [Y = NH; n = 0; X = 3-BrC6H4; R1 = R4 = H; R2 = MeC.tplbond.CC(O)NH; R3 = MeO] which showed IC50 of 0.15 .mu.M against epidermal growth factor receptor kinase (A431 membrane ext.).

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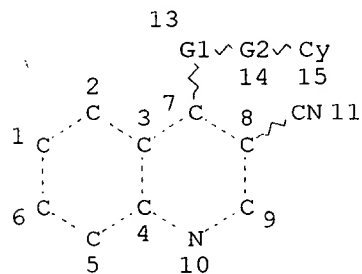
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L5 HAS NO ANSWERS

L5 STR



VAR G1=O/N/S  
 REP G2=(0-1) CH2  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: